Nuclear Criticality Safety Engineer Training
Module 7 [1]

The Monte Carlo Method - Introduction

LESSON OBJECTIVE

To introduce the theory of the Monte Carlo method. This is intended to lay the foundation for the KENO, MCNP and other stochastic codes used in criticality safety.

REFERENCES

There are many papers and books on the Monte Carlo method. The following is a list of a few references.

1. L. L. Carter and E. D. Cashwell, "Particle-Transport Simulation with the Monte Carlo Method," TID-26607, USERDA, 1975. (Probably out of print - a small book but a good introduction. Most of the material in this module on probability distribution functions is from this reference.)

2. N. M. Schaeffer, "Reactor Shielding for Nuclear Engineers," TID 25951, USAEC, 1973. (Chapter 5 is a good basic introduction to the topic.)

3. M. H. Kalos and P. A. Whitlock, "Monte Carlo Methods, Vol I: Basics," John Wiley and Sons, 1986. (This book has a good section on probability and the use of random numbers.)

4. I. Lux and L. Koblinger, "Monte Carlo Particle Transport Methods: Neutron and Photon Calculations," CRC Press, Boca Raton, FL, 1991. (A comprehensive text which includes many references and a section on criticality calculations.)

INTRODUCTION

The following six paragraphs are quoted from Reference 3.

> The name "Monte Carlo" was first applied to a class of mathematical problems by scientists working on the development of nuclear weapons in Los Alamos in the

[1] Developed for the U. S. Department of Energy Nuclear Criticality Safety Program by T. G. Williamson, Ph.D., Westinghouse Safety Management Solutions, Inc., in conjunction with the DOE Criticality Safety Support Group.

1940s. The essence of the method is the invention of games of chance whose behavior and outcome can be used to study some interesting phenomena. While there is no essential link to computers, the effectiveness of numerical or simulated gambling as a serious scientific pursuit is enormously enhanced by the availability of modern digital computers.

It is interesting, and may strike some as remarkable, that carrying out games of chance or random sampling will produce anything worthwhile. Indeed some authors have claimed that Monte Carlo will never be a method of choice for other than rough estimates of numerical quantities.

Perhaps the first documented use of random sampling to find the solution to an integral is that of Comte de Buffon. In 1777 he described the following experiment. A needle of length L is thrown at random onto a horizontal plane ruled with straight lines a distance d (d > L) apart. What is the probability P that a needle will intersect one of the lines? Comte de Buffon performed the experiment of throwing the needle many times to determine P. He also carried out the mathematical analysis and showed that $P = 2L/\pi d$.

Lord Kelvin appears to have used random sampling to aid in evaluating some time integrals of the kinetic energy that appear in the kinetic theory of gases. His random sampling consisted of drawing numbered pieces of paper from a bowl. He worried about the bias introduced by insufficient mixing of the papers and by static electricity.

In the 1930s Enrico Fermi made numerical experiments that would now be called Monte Carlo calculations. In studying the behavior of the newly discovered neutron, he carried out sampling experiments about how a neutral particle might be expected to interact with condensed matter. These led to substantial physical insight and to the more analytical theory of neutron diffusion and transport.

During the Second World War, the bringing together of such people as Von Neumann, Fermi, Ulam, and Metropolis at Los Alamos and the beginnings of modern digital computers gave strong impetus to the advancement of Monte Carlo. In the late 1940s and early 1950s there was a surge of interest. Unfortunately the computers of the time were not really adequate to carry out more than pilot studies in many areas.

Much of the early work was done at Oak Ridge and Los Alamos and has led to two "competing" families of codes. The 05R, MORSE and KENO series of codes were developed primarily at Oak Ridge and the MCNP family was developed at Los Alamos. The recent advances in computing technology, including faster personal computers, have allowed the Monte Carlo techniques to be applied to increasingly complicated problems.

A SIMPLE EXAMPLE

Play a simple game of tossing darts at a square board that has an inscribed circle. With a no-skill player (random tossing) what fraction of the darts falls in the circle? Calculate the area, A, of a circle with radius 1 inscribed in a square. Next consider the quadrant of the square containing positive x and positive y values less than or equal to 1.0. Randomly select values of x and y in the ranges $0 < x < 1$ and $0 < y < 1$ (i.e., measure the x and y positions of the randomly thrown darts). If $(x^2 + y^2) < 1$ a dart has landed in the circle and has scored; if not toss another dart to determine a new pair of random numbers. The ratio of the scores to the number of trials is the ratio of the area of the quadrant of the circle to the area of the square.

$$\frac{\text{SCORES}}{\text{TRIALS}} = \frac{(\pi / 4) * 1^2}{1^2} = \frac{\pi}{4}$$

Accumulate a large number of ratios of scores-to-trials, multiply by 4 and the result should be pi.

Here is a simple program in BASIC to compute this problem.

```
        'Program to find pi from the area of a circle inscribed in a square
        'The square is in the positive x and y quadrant with sides = 1
        PI=3.1415926
        RANDOMIZE TIMER
        T1=TIMER
        INPUT "NUMBER OF TRIALS", N
        FOR I = 1 TO N
        X = RND: Y = RND
        IF X^2 + Y^2 > 1 THEN GOTO 100
        N1=N1+1
100     NEXT I
        PI2=4*N1/N
        ERR=ABS((PI-PI2)/PI)*100
        PR=100*SQR(N1)/N1
        T2=TIMER: LT=T2-T1
```

In this program the randomize timer instruction starts a different random number sequence for each run and the timer instructions calculate the computer time. With some print statements included this program produced the results shown in the following table on an old (pre-pentium chip) computer.

The table lists the computed value of pi for each number of trials, the error, the precision and the computer time. The error is the difference between the computed value and the true value (in this case the true value is well-known), and the precision is a reflection of the accuracy of the calculation. Note that a precise calculation may have a large error if the calculation has not been properly done. In this case the error and the precision show similar trends. This example is given

to illustrate the point that the more cases that are run the smaller the error, the better the precision and the more costly in computer time.

Number of trials	PI	% Error	% Precision	Time (s)
100	3.040	3.23	11.47	4.2
100	3.880	8.33	11.79	3.6
1000	2.996	4.63	3.65	15.0
1000	3.140	0.05	3.57	13.1
2000	3.184	1.35	2.51	24.6
2000	3.172	0.97	2.51	24.4
5000	3.097	1.43	1.61	56.8
10000	3.152	0.34	1.13	109.8
10000	3.136	0.18	1.13	109.7

This example is sometimes given as a routine to generate the value of pi. It also is an example of a routine to evaluate the integrals

$$\int_0^1 dx \int_0^{\sqrt{1-x^2}} dy = \int_0^1 \sqrt{1-x^2}\, dx = \frac{\pi}{4}$$

or

$$\int_0^{\pi/2} d\varphi \int_0^1 dr = \frac{\pi}{4} \ .$$

The efficiency of this algorithm is $\pi/4 = 0.785$, which is to say that 78% of the random numbers contribute to the score.

A COMMENT ON STATISTICS

In a Monte Carlo simulation of radiation transport, whether it is for a shielding application, the calculation of the response of a radiation detector, the calculation of the absorption, leakage and fission rates in a multiplying assembly, the computation of pi or the evaluation of integrals, we must be aware of the number of events that contribute to the score. In nuclear engineering laboratory courses the students are taught that the relative one-standard-deviation (1σ) uncertainty in a counting experiment is

$$\sqrt{N} \ / \ N$$

where N is the number of counts recorded. The students are often urged to count until they had accumulated at least 10,000 counts so the relative uncertainty is at least 1%. If you have an answer with an uncertainty of 10% and an uncertainty of 1% is desired, then 100 times as many events must be counted.

A one-sigma uncertainty means that, if the distribution of values is normally distributed, on the average about 67% of the results should be within one standard deviation of the average of all of the values. If the experiment is repeated many times, the average of the results should approach the true result of the experiment. Approximately two-thirds of the measured results should be within one standard deviation of the mean and one-third of the results should be outside of this range.

Consider a one-dimensional shielding calculation in which the number of particles transmitted is the score. For a parallel radiation beam the transmission fraction is exp(-t), where t is the shield thickness in mean free paths. To have a 3% uncertainty in the score, i.e., 1000 transmitted events, how many particles must be started?

Thickness (mfp)	Transmission Fraction	Number started
1	0.368	2.7×10^3
2	0.135	7.4×10^3
3	0.0498	2.0×10^4
5	0.0067	1.5×10^5
8	0.00033	3.0×10^6
10	0.000045	2.2×10^7

That is, for a thick shield, 10 mean free paths, 22 million particles would have to be started toward the shield to achieve a 3% uncertainty in the number of transmitted particles.

SAMPLING FROM A PROBABILITY DISTRIBUTION FUNCTION

Introduce the *Probability Density Function* (PDF), f(x), which describes the relative frequency of occurrences of a random variable x. Its domain (all possible values of x) constitutes the event space. The PDFs are also called *frequency functions* or *probability distributions*. (Note the lower case notation, f(x), for the PDF.)

Let

$$P(x < x_0 < x+\delta x)$$

be the differential probability that the random variable x_0 lies within the interval $\{x, x+\delta x\}$. For a full range $\{a,b\}$ of the variable x, the probability that x lies in the interval $\{a,b\}$ is

$$P(a < x < b) = \int_a^b f(x)dx$$

This implies two properties of f(x):

$$f(x) \geq 0$$

and

$$\int_{-\infty}^{+\infty} f(x)dx = 1 \ .$$

The first relation is a statement that the probabilities must be positive and the second states that the probability of finding the chosen event somewhere in event space is unity.

Introduce the *Cumulative Density Function* (CDF), F(x), which is the probability that a random variable, x, has a value less than or equal to some fixed value. (Note the upper case notation for the CDF.)

$$F(x_0) = P(x \leq x_0) = \int_{-\infty}^{x_0} f(x)dx$$

with the restrictions that

$$\lim_{x \to -\infty} F(x) = 0$$

and

$$\lim_{x \to \infty} F(x) = 1 \ .$$

The PDF can be calculated from the CDF.

$$P(a < x < b) = \int_a^b f(x)dx = F(a) - F(b)$$

Let n be a random number equally distributed in the interval $\{c,d\}$ and let g(n) be the probability distribution function of n with a cumulative distribution function

$$G(n) = \int_c^n g(n')dn'$$

(Note that the integral is restricted to the domain of n.) Since n is expected to be uniformly distributed, choose the PDF to be a constant,

$$g(n) = \frac{1}{d - c}$$

so that

$$G(n) = \frac{1}{d - c}\int_c^n dn' = \frac{n - c}{d - c} \ .$$

An obvious choice of values is (c = 0) and (d = 1) so that G(n) = n. To relate the random variable n to an arbitrary value x

$$f(x)dx = g(n)dn$$

and

$$F(x) = G(n) = n$$

or

$$\int_a^b f(x)dx = \int_c^d g(n)dn = G(n) = n \ .$$

EXAMPLES

1) The probability distribution function f(x) is a constant, k, in the interval {0,1}. Then

$$f(x) = k$$

and

$$F(x) = n = \frac{\int_0^x f(x')dx'}{\int_0^1 f(x')dx'} = \frac{\int_0^x kdx'}{\int_0^1 kdx'} = \frac{kx}{k} = x$$

Thus the value of x is the random number n. Note that the integral in the denominator is necessary to normalize the CDF to meet the criterion given earlier that F(x) = 1 at the limit of its interval, x = 1.

2) The probability distribution function f(x) is a constant, k, in the interval {-1,1}. Then f(x) = k and

$$F(x) = n = \frac{\int_{-1}^x kdx'}{\int_{-1}^{+1} kdx'} = \frac{x + 1}{2}$$

and

$$x = 2 * n - 1$$

Note that when the random number n = 0, x = -1 and when n = 1, x = 1.

3) The distribution f(θ) is a constant, k, in the interval {0,2π}. Then f(θ) = k and

$$F(\theta) = n = \frac{\int_0^{\theta} k d\theta'}{\int_0^{2\pi} k d\theta'} = \frac{\theta}{2\pi}$$

and

$$\theta = 2\pi * n$$

4) The neutron scattering angular distribution is σ(θ). The CDF for this distribution is

$$F(\theta_0) = n = \frac{\int_0^{\theta_0} \sigma(\theta)\sin(\theta)d\theta}{\int_0^{\pi} \sigma(\theta)\sin(\theta)d\theta}$$

where n is a random number. In this case the functional relation for the cross section must be known or a numerical technique must be used to evaluate these integrals. It may be possible to evaluate the integrals and use a table lookup to determine the scattering angle.

REJECTION METHOD

This procedure that has been outlined so far is okay if f(x) is known and F(x) can be calculated. Another approach is the rejection technique which is useful if F(x) is not easily calculable, i.e., the integral cannot be easily evaluated.

For f(x) defined in the interval {a,b} choose two random numbers, n_1 and n_2. Locate a coordinate, x_1 in the range

$$x_1 = a + n_1 * (b - a)$$

and calculate

$$N = n_2 * K$$

where K is the maximum value of the function in the range {a,b}. This sets the condition that the function must be bounded in the interval.

If $N > f(x_1)$ then the number is rejected and another pair of random numbers is selected. The pairs of numbers which are retained fill in the area under the curve, and the integral of the function has been evaluated. This is exactly what was done in the first example of calculating the value of pi.

EXAMPLE

Use the rejection concept to find values of the sine and cosine. Select a pair of random numbers, n_1 and n_2. Compute

$$x_1 = 2*n_1 - 1$$

and

$$x_2 = 2*n_2 - 1$$

so that x_1 and x_2 are equally distributed in the range {-1,1}. If $(x_1^2 + x_2^2 < 1)$ then the points are inside a circle inscribed in the square and are retained. If not a new pair of random numbers is chosen. Then

$$\cos\theta = \frac{x_1}{\sqrt{x_1^2 + x_2^2}}$$

$$\sin\theta = \frac{x_2}{\sqrt{x_1^2 + x_2^2}}$$

The efficiency of this routine is the ratio of the circle area to the square area, $\pi/4 = 0.78$, which is very good.

To this point we have introduced the mathematics of the Monte Carlo technique and given examples of evaluating simple integrals. Remembering that the neutron transport equation is an integral equation it is suggested that this equation might be solvable by the Monte Carlo technique.

RADIATION TRANSPORT

The general solution the radiation transport problem by Monte Carlo in simple terms is accomplished by following the history of each individual particle by describing each event in the life of the particle in probabilistic terms. In principle each particle is followed until it disappears and some type of scoring is done for each event. In practice this procedure can be wasteful of computer time and fair games are played to maximize the amount of information learned from each history.

The problem of radiation transport will be described in three components: source characterization, transport and interactions, and scoring. It will start with a simple description of each component of the problem to illustrate the process and then include a brief discussion of weighting schemes to speed up the procedures.

SOURCE CHARACTERIZATION

To characterize the source properly, the following must be known.

Type of particles
Geometry
Angular distribution
Energy distribution.

(Note that when the source has been characterized, six of the seven parameters in the transport equation of NCSET Module 6 are determined; i.e., position (x,y,z), direction (θ,φ) and energy (E), all of the seven parameters except time.

Type of particle

Knowing the type of particle is an obvious place to start and determines the extent of the cross section libraries needed. For criticality problems we are primarily concerned with neutrons and rarely worry about other particles. However, if the criticality specialist is concerned with the dose to personnel, as for example in determining evacuation routes and exclusion zones, or in determining the response of criticality detectors, then the transmission of gamma rays or charged particles may also be of interest. Some Monte Carlo codes include coupled neutron-photon transmission in which neutron capture reactions are the sources of gamma rays. Other codes include charged particle transport and can be coupled with gamma-ray transport to determine the source of the charged particles.

Geometry

The following are some simple examples of locating the source starting position:.

Example A: *Particles are uniformly distributed on the surface of a circular disk of radius R*

In Cartesian coordinates, choose two random numbers n_1 and n_2 and find the x and y coordinates.

$$x = R(2 * n_1 - 1)$$
$$y = R(2 * n_2 - 1)$$

If ($x^2 + y^2 \# R^2$), then this point is on the disk. This routine has an efficiency of 78%, requires two random numbers and one decision.

In polar coordinates, choose two random numbers n_1 and n_2. The probability distribution for the radial position, p(r), is

$$p(r) = 2\pi r$$

and the cumulative distribution function, P(r), is

$$P(r) = n_1 = \frac{\int_0^r 2\pi r' dr'}{\int_0^R 2\pi r' dr'} = \frac{r^2}{R^2} \ .$$

Thus the radial position is chosen from the distribution

$$r = R\sqrt{n_1}$$

The distribution for the angular position, $p(\theta) = K$, where K is a constant and the cumulative distribution function $P(\theta)$ is

$$P(\theta) = n_2 = \frac{\int_0^\theta K d\theta'}{\int_0^{2\pi} K d\theta'} = \frac{\theta}{2\pi}$$

and the angular position is chosen from the distribution

$$\theta = 2\pi n_2 \ .$$

This routine has an efficiency of 100% and requires two random numbers and no decisions, but requires the time consuming square root operation for the radial position.

Example B: *Particles uniformly distributed in a spherical volume of radius R*

The distribution is a constant, K, and each of the three coordinates are calculated independent of one another, which means that three random numbers are required. The distribution function is weighted by the volume element

$$dV = r^2 dr \sin(\theta) d\theta d\varphi$$

so the cumulative distribution functions are

$$P(r) = n_1 = \frac{\int_0^r r'^2 dr'}{\int_0^R r'^2 dr'} = \frac{r^3}{R^3}$$

$$P(\theta) = n_2 = \frac{\int_0^\theta \sin\theta' d\theta'}{\int_0^\pi \sin\theta' d\theta'} = \frac{1 - \cos\theta}{2}$$

$$P(\varphi) = n_3 = \frac{\int_0^{\varphi} d\varphi'}{\int_0^{2\pi} d\varphi'} = \frac{\varphi}{2\pi}$$

The position coordinates are chosen from

$$r = R * \sqrt[3]{n_1}$$
$$\theta = \cos^{-1}(1 - 2 * n_2) \cdot$$
$$\varphi = 2\pi n_3$$

Normally it is not necessary to calculate the inverse cosine since the direction cosine appears in most of the calculations. With

$$\mu = \cos\theta$$

then

$$\mu = 1 - 2 * n_2 \cdot$$

Angular Distribution

One choice is to choose the direction vector, Ω, for the particle. Let this vector be specified by the polar angle, θ, and the azimuthal angle, ϕ (not to be confused with the spherical coordinate positions of Example B above). If the distribution is isotropic, the frequency distribution is a constant, K, and the cumulative distribution for the polar angle is

$$P(\theta) = n = \frac{\int_0^{\theta} \sin\theta' d\theta'}{\int_0^{\pi} \sin\theta' d\theta'} = \frac{1 - \cos\theta}{2} \cdot$$

Again, it is not necessary to calculate the inverse cosine since the direction cosine appears in most of the calculations. The azimuthal angle is chosen, with another random number, from a uniform distribution over the range $0 \# \phi \# 2\pi$.

In this example the integration has been over the full range of the angular variables but in some cases it may be expedient to limit the range. For example, in a problem in which particles are started at the origin of the coordinate system located on the surface of a slab shield, it is convenient to locate the z coordinate normal to the slab and limit the range of θ from 0 to $\pi/2$. Then the range of $\cos\theta$ is 0 to 1.0 and $\cos\theta$ = n, a random number. Thus all of the particles are moving into the slab and computer time is not wasted on particles which can never interact in the shield. However, you must remember that you are now dealing with only half of the particles and the source strength must be adjusted accordingly.

Energy Distribution

An obvious simple case is that of monoenergetic particles, for example a radioisotope that emits only a single-energy photon. An extension of this would be to calculate a series of monoenergetic cases and then sum the results of many computations with proper weighting for the true source distribution. Another approach is to integrate over a frequency distribution which describes the source. As an example, consider a ^{235}U fission source for which the energy spectrum can be described by this frequency distribution

$$p(E) = 0.4527 e^{E/0.965} \sinh\sqrt{2.29E}$$

with $0 < E < 20$ MeV. The cumulative distribution function is

$$P(E) = n = \frac{\int_0^E p(E')dE'}{\int_0^{20} p(E')dE'} = \int_0^E p(E')dE'$$

since the distribution is normalized. This integral is not easily evaluated; however, it can be evaluated numerically and tabulated. A table lookup routine with proper interpolation might be the way to select from this distribution or it could be integrated with the rejection technique.

PATH LENGTH

Let μ be the total interaction cross section. In the case of neutrons the notation is often Σ, the total macroscopic cross section. Remember that the total cross section includes all types of interactions: scattering, absorption, fission, etc. The probability per unit path of a particle interacting at a path length L is

$$p(L) = \mu e^{-\mu L}$$

and the cumulative distribution is

$$P(L) = n = \frac{\int_0^L \mu e^{-\mu L'} dL'}{\int_0^\infty \mu e^{-\mu L'} dL'} = 1 - e^{-\mu L}$$

The path length is then

$$L = -\frac{1}{\mu}\ln(1 - n) = -\frac{1}{\mu}\ln(n)$$

where the last step is made because the random number, n, and (1 - n) are equally distributed.

If the particle started at position x_0, y_0, and z_0, its new location is

$$x = x_0 + L \sin\theta \cos\phi$$

$$y = y_0 + L \sin\theta \sin\phi$$

$$z = z_0 + L \cos\theta$$

where θ and ϕ are the initial polar and azimuthal angles for the particle. The question is now asked, “Are the coordinates x, y and z within the boundaries of interest?" If a boundary between regions with different material properties has been crossed, the particle is placed at the boundary and a path length is calculated for the cross sections of the new region. If the particle has escaped from all regions of interest, it is scored as a leakage particle and another particle is started. Note that if the particle is scored we also have knowledge of its direction and energy, which may be useful.

If the particle is in a region of interest the next question is "What is the fate of the particle?" List the types of interactions which may occur and make a choice. For example, a neutron might scatter, it might interact in a fission event, or it might be captured in a nonfission interaction. In this case

$$\mu = \mu_s + \mu_c + \mu_f$$

Now choose two random numbers, n_1 and n_2, and make the following decisions.

If $n_1 \ \# \mu_s / \mu$ then a scatter occurs;

if not, then if $n_2 \ \# \mu_f / (\mu_f + \mu_c)$ then a fission occurs, else a nonfission capture occurs.

This procedure requires two random numbers and two choices. A different procedure which requires one random number, n, but three choices is to make the following decisions.

If $n \ \# \mu_s / \mu$ then a scatter occurs;

else if $\mu_s / \mu < n \ \# (\mu_s + \mu_f) / \mu$ then a fission occurs;

else if $(\mu_s + \mu_f) / \mu < n \ \# 1$, then a capture occurs.

This procedure is most efficient if the first choice is the most likely.

If the event is a nonfission capture the history could be terminated or a secondary particle, such as a capture gamma ray could be born at the location and followed. It may be important to know more about the nature of the capture, for example the isotope in which the capture occurs by choosing a random number and making a decision based on the ratio

$$\frac{\mu_c^j}{\sum_j \mu_c^j}$$

where the index j includes all isotopes which capture neutrons.

If the event is a fission, a choice based on cross section ratios is made about which isotope fissions and then fission neutrons are started at this point. The process will be repeated ν times for each neutron produced in the fission event. For each fission neutron a new starting direction and energy must be chosen.

If the event is a scatter, the isotope is chosen from the ratio of the scattering cross sections, the new direction vector is chosen from the scattering angular distribution, the new energy is calculated for this scattering angle, the total cross section at this energy is determined and the particle is sent on its way.

The frequency distribution for the angular distribution is the differential scattering cross section $\sigma(\theta)$, where θ is the scattering angle in the laboratory system. The azimuthal angle, ϕ, is chosen from a uniform distribution in the interval 0 to 2π. These scattering angles are relative to the direction of the incoming particle, so direction cosines relative to the original coordinate system must be computed. If (α, β, γ) are the direction cosines of the incident particle, the direction cosines of the scattered particle (α', β', γ') are given by the set of equations:

$$\alpha' = \alpha\cos\theta + \gamma\alpha\frac{\sin\theta\cos\phi}{\sqrt{1-\gamma^2}} - \beta\frac{\sin\theta\sin\phi}{\sqrt{1-\gamma^2}}$$

$$\beta' = \beta\cos\theta + \gamma\beta\frac{\sin\theta\cos\phi}{\sqrt{1-\gamma^2}} + \alpha\frac{\sin\theta\sin\phi}{\sqrt{1-\gamma^2}}$$

$$\gamma' = \gamma\cos\theta - \sqrt{1-\gamma^2}\sin\theta\cos\phi$$

except in the case where $(1 - \gamma^2)$ approaches zero, in which case the degenerate form

$$\alpha' = \alpha\sin\theta\cos\phi$$
$$\beta' = \beta\sin\theta\sin\phi$$
$$\gamma' = \gamma\cos\theta$$

is used.

The scattered particle then proceeds on its merry way in the new direction, with a new energy and a new set of cross sections. It may be prudent to place a lower limit on the energy of the particle so computer time is not wasted with low importance particles.

Up to this point a particle has been followed until it escapes the region of interest, is absorbed, or scatters to some energy so low that interest is lost. The history may have included the tracing of secondary particles but eventually the fates of the particle and its secondaries are scored, and a new particle is started. This description has been a "brute force" approach and the next step is to review the procedure with the thought in mind of improving the efficiency.

IMPORTANCE SAMPLING

This module will close with a simple example of a weighting technique which gives higher weights to particles in important regions and lower weights to particles in less important regions.

Suppose there is an isotropic source at point A in a scattering medium and a detector at point B separate from A but also in the scattering medium. Particles which start from A in the general direction of B will have a greater chance of arriving at B than particles starting in other directions. Suppose we sample 10,000 particles of which we would expect 2000 to be in the solid angle $d\Omega$ where they would have a greater chance of arriving at the detector and 8000 are starting in other directions. Some of those in the 8000 group may arrive at the detector so they *cannot be* ignored.

To increase the number which may score, suppose we force 6000 particles to start in $d\Omega$, give them a weight of 1/3 and give the remaining 4000 particles a weight of 2. The two situations are shown in the following table.

	Unbiased		Biased	
	Number	Weight	Number	Weight
In $d\Omega$	2000	1	6000	1/3
Outside	8000	1	4000	2
Total	10000		10000	

In the unbiased case all particles have weight of 1.0 for all values of Ω. In the biased case, three times as many particles are forced to start in a direction favoring interaction with detector B, but they are given a weight of 1/3, and half as many particles with weight 2.0 are started in other directions. The contribution to the final number of scores is

$$N = k\sum_{i=1}^{10000} w_i$$

where w_i is the weight for each event striking the detector (1/3 or 2) and k is a source normalization constant (e.g., 1/10,000).

Another rather obvious weight routine is to change the weight of a particle after each interaction so that the history is not lost when it is absorbed. At the location of each interaction score an absorption with a weight μ_a/μ and a scattering with weight $w = \mu_s/\mu$. The scattered particle weight is carried with the particle to the next interaction. It is not wise to carry the particle until the weight is so small that it will not contribute to each score so a lower limit is normally placed on the weight and the history is terminated when that limit is reached.

There are many other weighting techniques to increase the efficiency of Monte Carlo calculations. The important point is that the weighting techniques must be fair and not bias the answer. Much effort has been spent to play the Monte Carlo games fairly.

At this point the number of neutrons produced by fission, the number of neutrons absorbed and the number leaked have been computed, so with the proper weighting the multiplication factor, k_{eff}, may be calculated.

SUMMARY

In these sections a brief overview of the Monte Carlo technique has been presented so the criticality specialist will have some idea what happens when a Monte Carlo code is run. Significant points are that: it is a statistical process and the answer will have an uncertainty associated with it; all important regions of the problem must be sampled; and the answer is no better than the model used to approximate the real situation.

PROBLEMS

1. Write a Monte Carlo code to calculate the transmission of a parallel beam of radiation through a slab of material which is one mean free path thick. A thickness of one mean free path means that in the attenuation function, $\exp(-\mu x)$, the product $\mu x = 1.0$. For this problem, the fraction of transmitted particles is $\exp(-1) = 0.3679$. Calculate the error and precision of the result computed by the Monte Carlo routine. Investigate the error and precision of the calculation for slabs of different thicknesses and for different numbers of trials.

2. In Problem 1 the particles were all started in the same direction, i.e., normal to the surface of the slab. For the next problem start the particles with an angular distribution which is isotropic with respect to the surface normal. An isotropic distribution in the polar angle means that the cosines of the angles between the starting directions and the surface normal are equally distributed. If the cosines of the start angles are equally distributed in the interval from 0 to 1 then the angles are isotropically distributed in the interval from 0 to $\pi/2$. Compare the transmitted fraction with the transmitted fraction for a parallel beam (Problem 1). Compute the angular distribution of the transmitted particles and compare it with the initial distribution.

SOLUTIONS

1. This solution includes a program written in QUICKBASIC. That language was chosen because of the author's familiarity with it and because QUICKBASIC is available on many PCs. Other languages are acceptable. In this program the instruction "randomize timer" starts each calculation with a different random number. Without this instruction every calculation would use the same string of random numbers and give the same result.

```
'calculate transmission of
'parallel beam through finite slab
'slab thickness M mean free paths
RANDOMIZE TIMER
M = 1
'the desired answer is R
R = EXP(-M)
FOR I = 1 TO 5000
L = - LOG(RND)
IF L > M THEN T = T + 1
NEXT I
E = 100 * (R - (T / I)) / R
P = 100 * SQR(T) / T
PRINT
PRINT USING "SLAB THICKNESS ##.## MEAN FREE PATHS"; M
PRINT USING "R IS  ##.####"; R
PRINT USING "TRANSMISSION IS ##.####"; T / I
PRINT USING " PERCENT ERROR ##.## %"; E
PRINT USING " PRECISION  ##.## %"; P
PRINT "FOR"; I; "CASES"
```

RESULTS OF SEVERAL CALCULATIONS

MFP	Transmission	Computed Transmission	Error (%)	Precision (%)	# Trials
1.00	0.3679	0.3546	3.60	5.31	1000
1.00	0.3679	0.3662	0.47	1.65	10000
1.00	0.3679	0.3663	0.44	0.74	50000
3.00	0.0498	0.0499	- 0.22	2.00	50000
3.00	0.0498	0.0498	0.06	1.42	100000
5.00	0.00674	0.00707	- 4.93	3.76	100000
5.00	0.00674	0.00655	2.79	3.91	100000
5.00	0.00674	0.00679	- 0.80	1.72	500000
7.00	0.00091	0.00082	9.64	4.93	500000

For these results the column headed Transmission is the expected answer, the Computed Transmission is the value calculated by the Monte Carlo routine, the Error is the percent difference between the two computed values, the Precision is the one standard deviation uncertainty of the Monte Carlo result, and the # trials is the number of particles started. These cases illustrate that the precision and the error should be about the same, that the thicker the shield, the more cases must be run to achieve a low precision and that this simple problem can be solved with a few lines of a programming.

2. This solution also includes a program written in QUICKBASIC. In this case TH is the direction cosine of each starting particle, the array DIST(10) accumulates the angular distribution of the transmitted particles, L1 is the particle path length and L the component of the path length normal to the slab surface. The results are written into a file SLAB0.TXT.

```
'calculate transmission of particles
'through finite slab - isotropic source
'slab M mean free paths
RANDOMIZE TIMER
DIM DIST(10)
OPEN "SLAB0.TXT" FOR OUTPUT AS #1
M = .1
'the parallel beam answer is R
R = EXP(-M)
FOR I = 1 TO 10000
TH = RND
L1 = -(1)*LOG(RND)
L = L1 * TH
```

```
IF L > M THEN T = T + 1
IF L < M THEN GOTO 50
X = INT(10 * TH)
DIST(X) = DIST(X) + 1
50 NEXT I
PRINT
E = 100 * (R - (T / I)) / R
P = 100 * SQR(T) / T
PRINT
PRINT #1, USING "SLAB THICKNESS ##.## MEAN FREE PATHS"; M
PRINT #1, USING "R IS  ##.####"; R
PRINT #1, USING "TRANSMISSION IS ##.####"; T / I
PRINT #1, USING " PERCENT DIFFERENCE ##.## %"; E
PRINT #1, USING " PRECISION  ##.## %"; P
PRINT #1, "FOR"; I; "CASES"
PRINT #1, USING " ##.##   ##.#####  ##.#####  ##.##%  ##.##% ###### "; M; R; T / I;
E; P; I
PRINT
PRINT #1, "THE ANGULAR DISTRIBUTION FOLLOWS"
PRINT
FOR J = 0 TO 9
DIST(J) = DIST(J) / T
PRINT #1, USING "##.# #.###"; J; DIST(J)
S = S + DIST(J)
NEXT J
```

RESULTS OF SEVERAL CALCULATIONS

MFP	Beam Transmission	Computed Transmission	Precision (%)	# Cases
0.10	0.9048	0.7207	0.37	100000
1.00	0.3679	0.1481	0.82	100000
2.00	0.1353	0.0374	1.64	100000
3.00	0.0498	0.0105	1.38	500000
5.00	0.0067	0.00095	3.24	1000000

For these cases the slab thickness was varied from 0.1 to 5 mean free paths. The beam transmission is the result for a parallel beam and the computed transmission is that for an isotropic source. It is not surprising that the isotropic source transmission is less that for the parallel beam because many particles have longer paths through the slab than the slab thickness. This result points to the importance of knowing the angular distribution of the source particles. The angular distributions of the transmitted particles are in the next table.

Angular Bin \ Thickness (mfp)	0.1	1	2	3	5
0	0.020	0.000	0.000	0.000	0.000
1	0.070	0.001	0.000	0.000	0.000
2	0.092	0.014	0.001	0.000	0.000
3	0.103	0.041	0.010	0.002	0.000
4	0.111	0.069	0.028	0.016	0.001
5	0.117	0.107	0.074	0.038	0.013
6	0.121	0.146	0.135	0.096	0.067
7	0.120	0.180	0.185	0.178	0.127
8	0.122	0.206	0.243	0.267	0.273
9	0.124	0.236	0.323	0.404	0.519

The angular distribution is tabulated in equal bins of increasing cosine of the angle with the slab normal, that is bin 9 has those particle with the cosines between 0.9 and 1.0, which are the particles traveling with small angles to the normal. Each distribution has been normalized to one particle transmitted. For an isotropic distribution each entry would be 0.1. These distributions point out that the thicker the shield the more the angular distribution of transmitted particles is peaked in the forward direction.